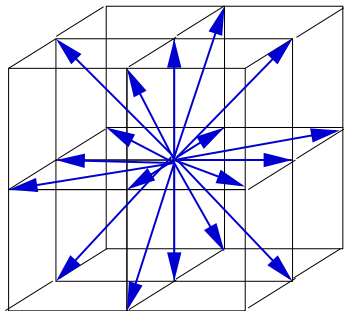


# Theory of the Lattice Boltzmann Method

Burkhard Dünweg  
Max Planck Institute for Polymer Research  
Ackermannweg 10  
55128 Mainz

B. D. and A. J. C. Ladd, arXiv:0803.2826v2,  
Advances in Polymer Science 221, 89 (2009)



- $\vec{c}_i$  small set of velocities
- $\vec{c}_i h$  connects two sites
- $n_i(\vec{r}, t)$ : real number, mass density on site  $\vec{r}$  corresponding to velocity  $\vec{c}_i$

- linearized Boltzmann equation (kinetic theory of gases)
- fully discretized
- sites  $\vec{r}$ , lattice spacing  $a$
- time  $t$ , time step  $h$

$$n_i(\vec{r} + \vec{c}_i h, t + h) = n_i^*(\vec{r}, t) = n_i(\vec{r}, t) + \Delta_i(\vec{r}, t)$$

# Conservation laws, symmetries

$$n_i(\vec{r} + \vec{c}_i h, t + h) = n_i^*(\vec{r}, t) = n_i(\vec{r}, t) + \Delta_i \{n_i(\vec{r}, t)\}$$

$$\rho = \sum_i n_i$$

$$\vec{j} = \rho \vec{u} = \sum_i n_i \vec{c}_i$$

$$\sum_i \Delta_i = \sum_i \Delta_i \vec{c}_i = 0$$



mass conservation



momentum conservation



locality



rotational symmetry (lattice!)



Galilei invariance (finite number of velocities)

# Low Mach number physics

- only  $u \ll c_i$
- only  $u \ll c_s$
- $Ma = u/c_s \ll 1$
- low Mach number  $\Rightarrow$  compressibility does not matter  $\Rightarrow$  equation of state does not matter  $\Rightarrow$  choose ideal gas!

$m_p$  particle mass:

$$p = \frac{\rho}{m_p} k_B T$$

$$c_s^2 = \frac{\partial p}{\partial \rho} = \frac{1}{m_p} k_B T$$

$$p = \rho c_s^2$$

$$k_B T = m_p c_s^2$$

# Where we want to get

in the continuum limit  $a \rightarrow 0$ ,  $h \rightarrow 0$ :

$$\partial_t \rho + \partial_\alpha j_\alpha = 0$$

$$\partial_t j_\alpha + \partial_\beta (\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta) = \partial_\beta \sigma_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \eta_{\alpha\beta\gamma\delta} \partial_\gamma u_\delta$$

$$\eta_{\alpha\beta\gamma\delta} = \left( \zeta - \frac{2}{3} \eta \right) \delta_{\alpha\beta} \delta_{\gamma\delta} + \eta (\delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma})$$

- $\eta$  shear viscosity
- $\zeta$  bulk viscosity

# Difference equation $\rightarrow$ differential equation

Example: consider

$$f(x + a) - f(x) = g(x)$$

small  $a$ :

$$a \frac{d}{dx} f(x) \approx g(x)$$

continuum limit  $a \rightarrow 0$ :

$$\frac{d}{dx} f(x) = \lim_{a \rightarrow 0} \frac{g(x)}{a}$$

watch out: if the rhs does not exist, then the continuum limit does not exist!

corrections to the leading behavior?

$$f(x+a) - f(x) = g(x)$$

set

$$D = a \frac{d}{dx}$$
$$g(x) = a(g_0(x) + ag_1(x) + a^2g_2(x) + \dots)$$

$g_i$  independent of  $a$

$$f(x_0+a) = f(x_0) + a \left. \frac{df}{dx} \right|_{x=x_0} + \frac{a^2}{2!} \left. \frac{d^2f}{dx^2} \right|_{x=x_0} + \dots$$
$$= \exp\left(a \frac{d}{dx}\right) f(x) \Big|_{x=x_0} = \exp(D) f(x) \Big|_{x=x_0}$$

$$\Rightarrow [\exp(D) - 1] f(x) = g(x)$$

$$f(x) = [\exp(D) - 1]^{-1} g(x)$$

$$Df(x) = D [\exp(D) - 1]^{-1} g(x)$$

now,

$$\frac{x}{\exp(x) - 1} = 1 - \frac{x}{2} + \frac{x^2}{12} - \frac{x^4}{720} + \frac{x^6}{30240} - + \dots = \sum_{k=0}^{\infty} \frac{B_k}{k!} x^k$$

Bernoulli numbers  $B_k$

$$\begin{aligned} f(x+a) - f(x) &= g(x) \Leftrightarrow \\ Df(x) &= \left[ 1 - \frac{D}{2} + \frac{D^2}{12} + \dots \right] g(x) \\ \frac{d}{dx} f(x) &= \left[ 1 - \frac{D}{2} + \frac{D^2}{12} + \dots \right] \\ &\quad [g_0(x) + ag_1(x) + a^2g_2(x) + \dots] \end{aligned}$$

systematic expansion in powers of  $a$ !



# LB continuum limit: how??

$a \rightarrow 0$ ,  $h \rightarrow 0$  to be replaced by  $\varepsilon \rightarrow 0$ :

- wave-like scaling:  $a/h = \text{const.}$

$$a = \varepsilon a_0$$

$$h = \varepsilon h_0$$

$$\vec{c}_i = \vec{c}_{i0}$$

$$n_i(\vec{r} + \varepsilon \vec{c}_{i0} h_0, t + \varepsilon h_0) - n_i(\vec{r}, t) = \Delta_i$$

- diffusive scaling:  $a^2/h = \text{const.}$

$$a = \varepsilon a_0$$

$$h = \varepsilon^2 h_0$$

$$\vec{c}_i = \varepsilon^{-1} \vec{c}_{i0}$$

$$n_i(\vec{r} + \varepsilon \vec{c}_{i0} h_0, t + \varepsilon^2 h_0) - n_i(\vec{r}, t) = \Delta_i$$

# Expanding the solution

lhs is  $O(\varepsilon) \Rightarrow$  rhs must be  $O(\varepsilon)$ !

ansatz:

$$\begin{aligned}n_i &= n_i^{(0)} + \varepsilon n_i^{(1)} + O(\varepsilon^2) \\ \Delta_i \{n_i\} &= \Delta_i^{(0)} + \varepsilon \Delta_i^{(1)} + O(\varepsilon^2) \\ &= \Delta_i \{n_i^{(0)}\} + \varepsilon \sum_j \left. \frac{\partial \Delta_i}{\partial n_j} \right|_{n_i=n_i^{(0)}} n_j^{(1)} + O(\varepsilon^2) \\ &=: \varepsilon \sum_j L_{ij} n_j^{(1)} + O(\varepsilon^2)\end{aligned}$$

and

$$\Delta_i \{n_i^{(0)}\} = 0$$

conservation laws:

$$\sum_i \Delta_i^{(k)} = \sum_i \Delta_i^{(k)} \vec{c}_i = 0$$

$$0 = \Delta_i^{(0)} = \Delta_i \{n_i^{(0)}\}$$

- $\{n_i^{(0)}\}$  collisional invariant,  $\{n_i^{(0)}\} = n_i^{eq}$
- no spurious conservation laws  $\Rightarrow$
- $n_i^{(0)} = n_i^{(0)}(\rho, \vec{j})$

# No expansion for conserved quantities!

$$n_i = n_i^{(0)} + \varepsilon n_i^{(1)} + O(\varepsilon^2)$$

$$\rho = \rho^{(0)} + \varepsilon \rho^{(1)} + O(\varepsilon^2)$$

$$\vec{j} = \vec{j}^{(0)} + \varepsilon \vec{j}^{(1)} + O(\varepsilon^2)$$

$$\begin{aligned} n_i^{(0)} &= n_i^{(0)}(\rho, \vec{j}) \\ &= n_i^{(0)}(\rho^{(0)} + \varepsilon \rho^{(1)} + O(\varepsilon^2), \vec{j}^{(0)} + \varepsilon \vec{j}^{(1)} + O(\varepsilon^2)) \end{aligned}$$

no expansion for  $n_i^{(0)} \Rightarrow$

$$\rho^{(1)} = \rho^{(2)} = \dots = 0$$

$$\vec{j}^{(1)} = \vec{j}^{(2)} = \dots = 0$$

i. e.



$$\rho^{(0)} = \rho$$



$$\vec{j}^{(0)} = \vec{j}$$



$$\sum_i n_i^{eq} = \rho$$



$$\sum_i n_i^{eq} \vec{c}_i = \vec{j}$$

- mass density

$$\rho = \sum_i n_i$$

- momentum density

$$j_\alpha = \sum_i n_i c_{i\alpha}$$

- stress

$$\Pi_{\alpha\beta} = \sum_i n_i c_{i\alpha} c_{i\beta}$$

- 3rd moment

$$\Phi_{\alpha\beta\gamma} = \sum_i n_i c_{i\alpha} c_{i\beta} c_{i\gamma}$$

$$n_i(\vec{r} + \varepsilon \vec{c}_i h_0, t + \varepsilon h_0) - n_i(\vec{r}, t) = \Delta_i$$

set

$$D_i = \varepsilon h_0 \partial_t + \varepsilon h_0 c_{i\alpha} \partial_\alpha$$

$$D_i n_i = \left[ 1 - \frac{D_i}{2} + \frac{D_i^2}{12} + \dots \right] \Delta_i$$

•  $\varepsilon^1$ :

$$(h_0 \partial_t + h_0 c_{i\alpha} \partial_\alpha) n_i^{(0)} = \Delta_i^{(1)}$$

•  $\varepsilon^2$ :

$$(h_0 \partial_t + h_0 c_{i\alpha} \partial_\alpha) n_i^{(1)} = \Delta_i^{(2)} - \frac{1}{2} (h_0 \partial_t + h_0 c_{i\alpha} \partial_\alpha) \Delta_i^{(1)}$$

take zeroth and first velocity moment:

- $\varepsilon^1$ :

$$\begin{aligned}h_0 \partial_t \rho + h_0 \partial_\alpha j_\alpha &= 0 \\h_0 \partial_t j_\beta + h_0 \partial_\alpha \Pi_{\alpha\beta}^{(0)} &= 0\end{aligned}$$

or

$$\begin{aligned}\partial_t \rho + \partial_\alpha j_\alpha &= 0 \\ \partial_t j_\beta + \partial_\alpha \Pi_{\alpha\beta}^{(0)} &= 0\end{aligned}$$

- $\varepsilon^2$ :

$$\begin{aligned}0 &= 0 \\ h_0 \partial_\alpha \Pi_{\alpha\beta}^{(1)} &= -\frac{1}{2} h_0 \partial_\alpha \left( \Pi_{\alpha\beta}^{(1)*} - \Pi_{\alpha\beta}^{(1)} \right)\end{aligned}$$

or

$$\frac{1}{2} \partial_\alpha \left( \Pi_{\alpha\beta}^{(1)*} + \Pi_{\alpha\beta}^{(1)} \right) = 0$$



consequences:

- $\Pi^{(0)}$  depends only on  $\rho, \vec{j}$  (locally!!)
- $\Rightarrow \Pi^{(0)}$  must be the Euler stress!
- i. e.

$$\sum_i n_i^{eq} c_{i\alpha} c_{i\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

- stress relaxation at order  $\varepsilon^2$  gives rise to “some sort of” dissipation, **but no relation** to the previous order
- i. e. relation to velocity gradients (viscous shear stresses) can not be established!
- we find: Euler equations at order  $\varepsilon^1$ , but no useful results beyond!

can we at least adjust  $n_i^{eq}$  such that we get Euler in the leading order? **YES!**

# The equilibrium populations

ansatz (Euler stress is a 2nd order polynomial in  $\vec{u}$ ):

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho (1 + A \vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + C u^2)$$

$w_i$  positive weights, identical within a shell. cubic symmetry:

$$\sum_i w_i = 1$$

$$\sum_i w_i c_{i\alpha} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} = \sigma_2 \delta_{\alpha\beta}$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = \kappa_4 \delta_{\alpha\beta\gamma\delta}$$

$$+ \sigma_4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma})$$

mass:

$$\begin{aligned}\rho &= \sum_i n_i^{eq} \\ &= \rho \sum_i w_i (1 + A\vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + Cu^2)\end{aligned}$$

$$\begin{aligned}0 &= Bu_\alpha u_\beta \sum_i w_i c_{i\alpha} c_{i\beta} + Cu^2 \\ &= Bu_\alpha u_\beta \sigma_2 \delta_{\alpha\beta} + Cu^2 \\ &= (B\sigma_2 + C) u^2\end{aligned}$$

$$C + B\sigma_2 = 0$$

momentum:

$$\begin{aligned}\rho u_\alpha &= \sum_i n_i^{\text{eq}} c_{i\alpha} \\ &= \rho \sum_i w_i c_{i\alpha} (1 + A\vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + Cu^2) \\ &= \rho A u_\beta \sum_i w_i c_{i\alpha} c_{i\beta} \\ &= \rho A u_\beta \sigma_2 \delta_{\alpha\beta} \\ &= \rho A \sigma_2 u_\alpha \\ A \sigma_2 &= 1\end{aligned}$$

stress:

$$\begin{aligned}c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta &= \frac{1}{\rho} \sum_i n_i^{eq} c_{i\alpha} c_{i\beta} \\ &= \sum_i w_i c_{i\alpha} c_{i\beta} (1 + A \vec{u} \cdot \vec{c}_i + B (\vec{u} \cdot \vec{c}_i)^2 + C u^2) \\ &= (1 + C u^2) \sigma_2 \delta_{\alpha\beta} + B u_\gamma u_\delta \kappa_4 \delta_{\alpha\beta\gamma\delta} \\ &+ B u_\gamma u_\delta \sigma_4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma})\end{aligned}$$

hence  $\kappa_4 = 0$  and

$$c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta = (\sigma_2 + C \sigma_2 u^2 + B \sigma_4 u^2) \delta_{\alpha\beta} + 2B \sigma_4 u_\alpha u_\beta$$

i. e.  $\sigma_2 = c_s^2$ ,  $C \sigma_2 + B \sigma_4 = 0$ ,  $2B \sigma_4 = 1$

taken all together:

$$\kappa_4 = 0$$

$$\sigma_2 = c_s^2$$

$$2B\sigma_4 = 1$$

$$C\sigma_2 + B\sigma_4 = 0$$

$$C + B\sigma_2 = 0$$

$$A\sigma_2 = 1$$

six equations, six unknowns. multiply Eq. 5 with  $\sigma_2$  and compare with Eq. 4. hence the solution is:

$$\kappa_4 = 0$$

$$\sigma_2 = c_s^2$$

$$\sigma_4 = c_s^4$$

$$A = 1/c_s^2$$

$$B = 1/(2c_s^4)$$

$$C = -1/(2c_s^2)$$

form of the equilibrium populations is

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho \left( 1 + \frac{\vec{u} \cdot \vec{c}_i}{c_s^2} + \frac{(\vec{u} \cdot \vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right)$$

what are the weights? we need to satisfy the three conditions:

$$\sum_i w_i = 1$$

$$\kappa_4 = 0$$

$$\sigma_4 = \sigma_2^2$$

therefore, at least three shells are needed! each shell is assigned its own  $\sigma_2$ ,  $\sigma_4$ ,  $\kappa_4$  (assuming weight one).

- one zero velocity:  $\vec{c}_i = 0$ , weight  $w_0$
- six nearest neighbors:  $\vec{c}_i = (a/h)(\pm 1, 0, 0)$ ,  $(a/h)(0, \pm 1, 0)$ ,  $(a/h)(0, 0, \pm 1)$ , weight  $w_I$
- twelve next-nearest neighbors:  $\vec{c}_i = (a/h)(\pm 1, \pm 1, 0)$ ,  $(a/h)(\pm 1, 0, \pm 1)$ ,  $(a/h)(0, \pm 1, \pm 1)$ , weight  $w_{II}$
- zeroth shell: velocity moments trivial



- first shell:

$$\sum_i c_{i1}^2 = 2(a/h)^2 = \sigma_2(l)$$

$$\sum_i c_{i1}^4 = 2(a/h)^4 = \kappa_4(l) + 3\sigma_4(l)$$

$$\sum_i c_{i1}^2 c_{i2}^2 = 0 = \sigma_4(l)$$

$$\sigma_2(l) = 2(a/h)^2$$

$$\sigma_4(l) = 0$$

$$\kappa_4(l) = 2(a/h)^4$$

- second shell:

$$\sum_i c_{i1}^2 = 8(a/h)^2 = \sigma_2(l)$$

$$\sum_i c_{i1}^4 = 8(a/h)^4 = \kappa_4(l) + 3\sigma_4(l)$$

$$\sum_i c_{i1}^2 c_{i2}^2 = 4(a/h)^4 = \sigma_4(l)$$

$$\sigma_2(l) = 8(a/h)^2$$

$$\sigma_4(l) = 4(a/h)^4$$

$$\kappa_4(l) = -4(a/h)^4$$

$$\begin{aligned}
0 &= \kappa_4 \\
&= w_I \kappa_4(I) + w_{II} \kappa_4(II) \\
&= 2w_I - 4w_{II} \\
w_I &= 2w_{II} \\
\sigma_2 &= w_I \sigma_2(I) + w_{II} \sigma_2(II) \\
&= w_{II} (2\sigma_2(I) + \sigma_2(II)) \\
&= w_{II} (a/h)^2 (2 \cdot 2 + 8) \\
&= 12w_{II} (a/h)^2 \\
\sigma_4 &= w_I \sigma_4(I) + w_{II} \sigma_4(II) \\
&= w_{II} (2\sigma_4(I) + \sigma_4(II)) \\
&= 4w_{II} (a/h)^4 \\
&= \sigma_2^2 \\
&= 144w_{II}^2 (a/h)^4
\end{aligned}$$

$$\begin{aligned}
 1 &= 36w_{II} \\
 w_{II} &= \frac{1}{36} \\
 w_I &= 2w_{II} = \frac{1}{18} \\
 1 &= w_0 + 6w_I + 12w_{II} \\
 &= w_0 + \frac{1}{3} + \frac{1}{3} \\
 w_0 &= \frac{1}{3} \\
 c_s^2 &= \sigma_2 \\
 &= 12w_{II}(a/h)^2 \\
 &= \frac{1}{3}(a/h)^2
 \end{aligned}$$

all coefficients of  $n_i^{eq}$  known!

# LB continuum limit: diffusive scaling

$$n_i(\vec{r} + \varepsilon \vec{c}_{i0} h_0, t + \varepsilon^2 h_0) - n_i(\vec{r}, t) = \Delta_i$$

watch out:  $\vec{c}_i = \varepsilon^{-1} \vec{c}_{i0}$ ! define moments wrt  $\vec{c}_{i0}$ , not  $\vec{c}_i$ ! e. g.  
 $\vec{j} = \sum_i n_i \vec{c}_{i0}$  etc.!

set:

$$D_i = \varepsilon^2 h_0 \partial_t + \varepsilon h_0 c_{i0\alpha} \partial_\alpha$$

$$D_i n_i = \left[ 1 - \frac{D_i}{2} + \frac{D_i^2}{12} + \dots \right] \Delta_i$$

•  $\varepsilon^1$ :

$$h_0 c_{i0\alpha} \partial_\alpha n_i^{(0)} = \Delta_i^{(1)}$$

•  $\varepsilon^2$ :

$$h_0 \partial_t n_i^{(0)} + h_0 c_{i0\alpha} \partial_\alpha n_i^{(1)} = \Delta_i^{(2)} - \frac{1}{2} h_0 c_{i0\alpha} \partial_\alpha \Delta_i^{(1)}$$

$$h_0 c_{i0\alpha} \partial_\alpha n_i^{(0)} = \Delta_i^{(1)}$$

zeroth velocity moment:

$$\partial_\alpha j_\alpha = 0$$

first velocity moment:

$$\partial_\alpha \Pi_{\alpha\beta}^{(0)} = 0$$

$$h_0 \partial_t n_i^{(0)} + h_0 c_{i0\alpha} \partial_\alpha n_i^{(1)} = \Delta_i^{(2)} - \frac{1}{2} h_0 c_{i0\alpha} \partial_\alpha \Delta_i^{(1)}$$

zeroth velocity moment:

$$\partial_t \rho = 0$$

incompressible fluid!

1st velocity moment:

$$\begin{aligned} \partial_t j_\beta + \partial_\alpha \Pi_{\alpha\beta}^{(1)} &= -\frac{1}{2} \partial_\alpha \left( \Pi_{\alpha\beta}^{(1)*} - \Pi_{\alpha\beta}^{(1)} \right) \\ \partial_t j_\beta + \frac{1}{2} \partial_\alpha \left( \Pi_{\alpha\beta}^{(1)*} + \Pi_{\alpha\beta}^{(1)} \right) &= 0 \end{aligned}$$

# Adding the equations

$$\begin{aligned}\partial_t \rho + \partial_\alpha j_\alpha &= 0 \\ \partial_t j_\beta + \partial_\alpha \Pi_{\alpha\beta}^{(0)} + \frac{1}{2} \partial_\alpha \left( \Pi_{\alpha\beta}^{(1)*} + \Pi_{\alpha\beta}^{(1)} \right) &= 0\end{aligned}$$

looks like Navier–Stokes;  $\Pi^{(0)}$  Euler stress,  $(1/2) (\Pi^{(1)*} + \Pi^{(1)})$  viscous stress; **BUT**

- dynamics with *constraints*:

$$\begin{aligned}\partial_\alpha j_\alpha &= 0 \\ \partial_\alpha \Pi_{\alpha\beta}^{(0)} &= 0 \\ \partial_t \rho &= 0\end{aligned}$$

- incompressible  $\rightarrow$  pressure as a Lagrange multiplier
- difficult to analyze! (Junk / Luo / Klar)



**All these difficulties go away when one combines wave-like and diffusive scaling in a multiple time scale analysis!**

So, what is this?

# The idea of multiple time scale expansion

example: damped oscillator

$$\frac{d^2}{dt^2}x + \frac{1}{\tau} \frac{d}{dt}x + \frac{1}{T^2}x = 0$$

- $T$  oscillation period
- $\tau$  frictional relaxation time
- consider  $T \ll \tau$  (weak damping)
- try to treat

$$\varepsilon := \frac{T}{2\tau}$$

as a small parameter for **perturbation theory**

- unit system: set  $T = 1$

$$\frac{d^2}{dt^2}x + 2\varepsilon \frac{d}{dt}x + x = 0$$

$$\frac{d^2}{dt^2}x + 2\varepsilon \frac{d}{dt}x + x = 0$$

- $x(t=0) = 1, \dot{x}(t=0) = -\varepsilon$
- exactly solvable

$$x(t) = \exp(-\varepsilon t) \cos\left(\sqrt{1 - \varepsilon^2}t\right)$$

$\varepsilon$  dependence looks harmless, **but** ...

$$\frac{d^2}{dt^2}x + 2\varepsilon \frac{d}{dt}x + x = 0$$

$$x(t) = x_0(t) + \varepsilon x_1(t) + \varepsilon^2 x_2(t) + \dots$$

yields hierarchy:

$$\ddot{x}_k + x_k = -2\dot{x}_{k-1}$$

with (def.)  $x_{-1} = 0$ , plus corresponding hierarchy of initial conditions

- $\varepsilon^0$ :

$$x_0 = \cos t$$

- $\varepsilon^1$ :

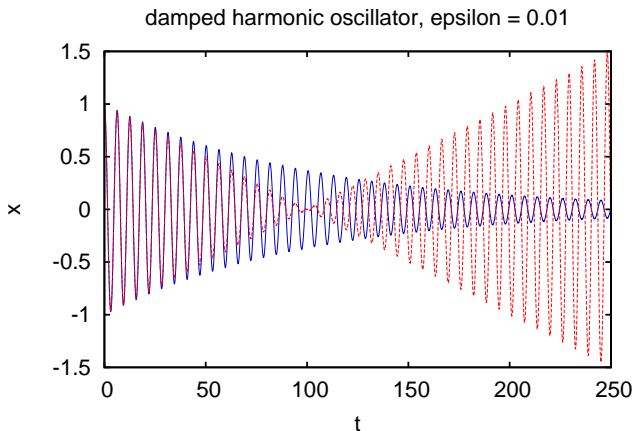
$$x_1 = -t \cos t$$

i. e., 1st order perturbation theory yields

$$x(t) = (1 - \varepsilon t) \cos t + O(\varepsilon^2)$$

identical with Taylor expansion of the exact solution!

**For  $t \gg 1/\varepsilon$  this becomes completely useless!!!**



## Deficiencies of naive perturbation theory:

- does not capture the presence of different time scales (here: fast oscillations vs. slow damping)
- typically, this occurs if one has *qualitatively different* behavior for  $\varepsilon = 0$  and small  $\varepsilon > 0$  (here: conservative vs. dissipative)
- “singular perturbation theory” needed

# Multiple time scale analysis

Idea:

$$\begin{aligned}x(t) &= \exp(-\varepsilon t) \cos\left(\sqrt{1-\varepsilon^2}t\right) \\ &\approx \exp(-\varepsilon t) \cos t \\ &= \exp(-t_1) \cos t \\ &= x(t, t_1)\end{aligned}$$

with

$$t_1 = \varepsilon t$$

consider  $x$  as a function of *two independent* variables  $t, t_1$

$\Rightarrow$  should be able to grasp the time scale separation!

hence, study expansion

$$x(t, t_1) = x_0(t, t_1) + \varepsilon x_1(t, t_1) + \varepsilon^2 x_2(t, t_1) + \dots$$

with

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{\partial t_1}{\partial t} \frac{\partial}{\partial t_1} = \frac{\partial}{\partial t} + \varepsilon \frac{\partial}{\partial t_1}$$

again the damped oscillator:

$$\begin{aligned}\frac{d}{dt}x &= p \\ \frac{d}{dt}p &= -2\varepsilon p - x\end{aligned}$$

(expand both  $x$  and  $p$ )

$\varepsilon^0$ :

$$\begin{aligned}\frac{\partial}{\partial t}x_0 &= p_0 \\ \frac{\partial}{\partial t}p_0 &= -x_0 \\ x_0 &= A(t_1) \cos t + B(t_1) \sin t \\ p_0 &= -A(t_1) \sin t + B(t_1) \cos t\end{aligned}$$

$A(t_1)$ ,  $B(t_1)$  not yet known



$\varepsilon^1$ :

$$\begin{aligned}\frac{\partial}{\partial t}x_1 &= p_1 - \frac{\partial}{\partial t_1}x_0 \\ \frac{\partial}{\partial t}p_1 &= -x_1 - \frac{\partial}{\partial t_1}p_0 - 2p_0\end{aligned}$$

ansatz

$$\begin{aligned}x_1 &= C(t, t_1) \cos t + D(t, t_1) \sin t \\ p_1 &= -C(t, t_1) \sin t + D(t, t_1) \cos t\end{aligned}$$

yields

$$\begin{aligned}\frac{\partial C}{\partial t} &= -\frac{\partial A}{\partial t_1} - 2A \sin^2 t + 2B \sin t \cos t \\ \frac{\partial D}{\partial t} &= -\frac{\partial B}{\partial t_1} - 2B \cos^2 t + 2A \sin t \cos t\end{aligned}$$

integrate wrt  $t$ , but the solution **should not explode!!!**

now,

$$\langle \sin^2 t \rangle = \langle \cos^2 t \rangle = \frac{1}{2}$$

hence

$$\frac{\partial A}{\partial t_1} + A = 0$$

$$\frac{\partial B}{\partial t_1} + B = 0$$

or

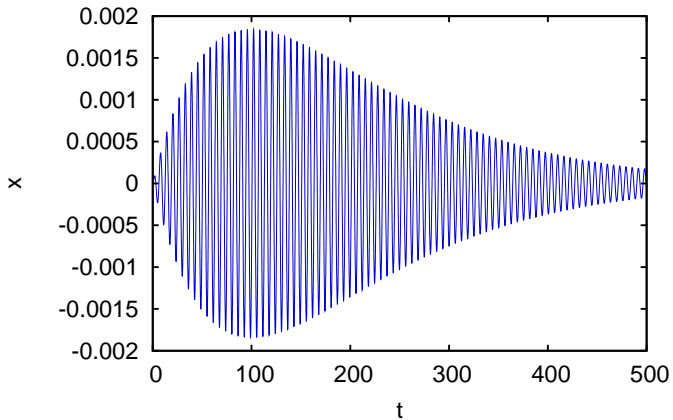
$$A = \hat{A} \exp(-t_1)$$

$$B = \hat{B} \exp(-t_1)$$

insert this into  $\varepsilon^0$  solution, initial conditions:

$$x_0 = \exp(-\varepsilon t) \cos t$$

difference exact vs. perturbation theory,  $\epsilon = 0.01$



# Chapman–Enskog expansion

- original LBE:

$$n_i(\vec{r} + \vec{c}_i h, t + h) - n_i(\vec{r}, t) = \Delta_i$$

- desired: continuum limit  $h \rightarrow 0$ ,  $\vec{c}_i$  fixed
- set  $h = \varepsilon h_0$
- expansion parameter  $\varepsilon \ll 1$ ,  $\varepsilon \rightarrow 0$
- write  $t_1 = t$ ,  $\vec{r}_1 = \vec{r}$
- yields:

$$n_i(\vec{r}_1 + \vec{c}_i \varepsilon h_0, t_1 + \varepsilon h_0) - n_i(\vec{r}_1, t_1) = \Delta_i$$

- two time scales:
  - waves: time  $\sim$  length
  - diffusion: time  $\sim$  (length)<sup>2</sup>
- second time scale:  $t_2 = \varepsilon t$

- study LBE:

$$n_i(\vec{r}_1 + \varepsilon \vec{c}_i h_0, t_1 + \varepsilon h_0, t_2 + \varepsilon^2 h_0) - n_i(\vec{r}_1, t_1, t_2) = \Delta_i$$

- 

$$\frac{\partial}{\partial \vec{r}} = \frac{\partial}{\partial \vec{r}_1}$$

- 

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_1} + \varepsilon \frac{\partial}{\partial t_2}$$

- set

$$D_i = \varepsilon h_0 c_{i\alpha} \partial_{1\alpha} + \varepsilon h_0 \partial_{t_1} + \varepsilon^2 h_0 \partial_{t_2}$$

$$D_i n_i = \left[ 1 - \frac{D_i}{2} + \frac{D_i^2}{12} + \dots \right] \Delta_i$$

- $\varepsilon^1$ :

$$(h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) n_i^{(0)} = \Delta_i^{(1)}$$

- $\varepsilon^2$ :

$$\begin{aligned} & h_0 \partial_{t2} n_i^{(0)} + (h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) n_i^{(1)} \\ = & \Delta_i^{(2)} - \frac{1}{2} (h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) \Delta_i^{(1)} \end{aligned}$$

or

$$h_0 \partial_{t2} n_i^{(0)} + \frac{1}{2} (h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) (n_i^{(1)*} + n_i^{(1)}) = \Delta_i^{(2)}$$

# Zerth velocity moment: Mass conservation

$$\partial_{t_1} \rho + \partial_{1\alpha} j_\alpha = 0$$

$$\partial_{t_2} \rho = 0$$

Hence,

👍 continuity equation OK!!!

# First velocity moment: Momentum conservation

$$\partial_{t_1} j_\alpha + \partial_{1\beta} \Pi_{\alpha\beta}^{(0)} = 0$$

$$\partial_{t_2} j_\alpha + \frac{1}{2} \partial_{1\beta} \left( \Pi_{\alpha\beta}^{*(1)} + \Pi_{\alpha\beta}^{(1)} \right) = 0$$

comparison with Navier–Stokes:

Euler stress:

$$\Pi_{\alpha\beta}^{(0)} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

Newtonian viscous stress:

$$\frac{\varepsilon}{2} \left( \Pi_{\alpha\beta}^{*(1)} + \Pi_{\alpha\beta}^{(1)} \right) = -\sigma_{\alpha\beta}$$



## Second velocity moment: A useful relation

$$\partial_{t_1} \Pi_{\alpha\beta}^{(0)} + \partial_{1\gamma} \Phi_{\alpha\beta\gamma}^{(0)} = h_0^{-1} \left( \Pi_{\alpha\beta}^{*(1)} - \Pi_{\alpha\beta}^{(1)} \right)$$

from explicit form of  $n_i^{eq}$ :

$$\Phi_{\alpha\beta\gamma}^{(0)} = \rho c_s^2 (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta})$$

use continuity and Euler for

$$\partial_{t_1} \Pi_{\alpha\beta}^{(0)} = \partial_{t_1} (\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta) = \dots$$

$\Rightarrow$  (neglecting terms  $O(u^3)$ ):

$$\Pi_{\alpha\beta}^{*(1)} - \Pi_{\alpha\beta}^{(1)} = h_0 \rho c_s^2 (\partial_\alpha u_\beta + \partial_\beta u_\alpha)$$

(details see next three slides)

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho \left( 1 + \frac{\vec{u} \cdot \vec{c}_i}{c_s^2} + \frac{(\vec{u} \cdot \vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right)$$

hence

$$\begin{aligned} \Phi_{\alpha\beta\gamma} &= \frac{\rho}{c_s^2} u_\delta \sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} \\ &= \frac{\rho}{c_s^2} u_\delta c_s^4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \\ &= \rho c_s^2 (\delta_{\alpha\beta} u_\gamma + \delta_{\alpha\gamma} u_\beta + \delta_{\beta\gamma} u_\alpha) \end{aligned}$$

# Equation of motion for the Euler stress

pure Euler hydrodynamics

$$\Pi_{\alpha\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

Euler equations:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_\gamma \partial_\gamma$$

$$\frac{D}{Dt} \rho = -\rho \partial_\gamma u_\gamma$$

$$\rho \frac{D}{Dt} u_\alpha = -c_s^2 \partial_\alpha \rho$$

$$\begin{aligned} \frac{D}{Dt} \Pi_{\alpha\beta} &= (c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta) \frac{D}{Dt} \rho + u_\alpha \rho \frac{D}{Dt} u_\beta + u_\beta \rho \frac{D}{Dt} u_\alpha \\ &= -\rho (c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta) \partial_\gamma u_\gamma - c_s^2 u_\alpha \partial_\beta \rho - c_s^2 u_\beta \partial_\alpha \rho \end{aligned}$$

neglect  $O(u^3)$ :

$$\frac{\partial}{\partial t} \Pi_{\alpha\beta} + u_\gamma c_s^2 \delta_{\alpha\beta} \partial_\gamma \rho = -c_s^2 \delta_{\alpha\beta} \rho \partial_\gamma u_\gamma - c_s^2 u_\alpha \partial_\beta \rho - c_s^2 u_\beta \partial_\alpha \rho$$

$$\begin{aligned}
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + c_s^2 \delta_{\alpha\beta} \partial_\gamma (\rho u_\gamma) + c_s^2 u_\alpha \partial_\beta \rho + c_s^2 u_\beta \partial_\alpha \rho = 0 \\
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + c_s^2 \delta_{\alpha\beta} \partial_\gamma (\rho u_\gamma) + c_s^2 \partial_\beta (\rho u_\alpha) + c_s^2 \partial_\alpha (\rho u_\beta) \\
= & c_s^2 \rho \partial_\beta u_\alpha + c_s^2 \rho \partial_\alpha u_\beta \\
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + \partial_\gamma \{ \rho c_s^2 (\delta_{\alpha\beta} u_\gamma + \delta_{\beta\gamma} u_\alpha + \delta_{\alpha\gamma} u_\beta) \} \\
= & c_s^2 \rho \partial_\beta u_\alpha + c_s^2 \rho \partial_\alpha u_\beta \\
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + \partial_\gamma \Phi_{\alpha\beta\gamma} = \rho c_s^2 (\partial_\alpha u_\beta + \partial_\beta u_\alpha)
\end{aligned}$$

$$\begin{aligned}\Delta_i &= \Delta_i^{(0)} + \varepsilon \Delta_i^{(1)} + O(\varepsilon^2) \\ &= \varepsilon \Delta_i^{(1)} + O(\varepsilon^2)\end{aligned}$$

$O(\varepsilon^2)$  does not contribute to hydrodynamics  $\Rightarrow$  ignore

$$\Delta_i^{(1)} = \sum_j \left. \frac{\partial \Delta_i}{\partial n_j} \right|_{\{n_k^0\}} n_j^{(1)} = \sum_j L_{ij} n_j^{(1)}$$

i. e.

$$\Delta_i = \sum_j L_{ij} (n_j - n_j^{eq})$$

# The linear collision process

$$n_i^{neq} := n_i - n_i^{eq}$$

$$n_i^* = n_i + \sum_j L_{ij} n_j^{neq}$$

$$n_i^{neq*} = n_i^{neq} + \sum_j L_{ij} n_j^{neq}$$

$$\Gamma_{ij} := \delta_{ij} + L_{ij}$$

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$\Gamma = ???$

simplest choice: Lattice BGK:

$$\Gamma_{ij} = \left(1 - \frac{1}{\tau}\right) \delta_{ij}$$

study here the MRT (multi relaxation time) framework!

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$$\sum_i \Rightarrow$$

$$0 = \sum_j \left( \sum_i \Gamma_{ij} \right) n_j^{neq}$$

$$0 = \sum_i \Gamma_{ij}$$

$$e_{0i} := 1$$

$$e_{0j} \cdot 0 = \sum_i e_{0i} \Gamma_{ij}$$

i. e.  $\vec{e}_0$  is left eigenvector, eigenvalue zero.

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$$\sum_i c_{ix} \Rightarrow$$

$$0 = \sum_j \left( \sum_i c_{ix} \Gamma_{ij} \right) n_j^{neq}$$

$$0 = \sum_i c_{ix} \Gamma_{ij}$$

$$e_{1i} := c_{ix}$$

$$e_{1j} \cdot 0 = \sum_i e_{1i} \Gamma_{ij}$$

i. e.  $\vec{e}_1$  is left eigenvector, eigenvalue zero.

analogous:  $e_{2i} = c_{iy}$ ,  $e_{3i} = c_{iz}$



$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$\sum_i c_{i\gamma} c_{i\gamma}$  (bulk stress)  $\Rightarrow$  (bulk stress relaxation with  $\gamma_b$ ):

$$\Pi_{\gamma\gamma}^{neq*} = \sum_j \left( \sum_i c_{i\gamma} c_{i\gamma} \Gamma_{ij} \right) n_j^{neq}$$

$$\Pi_{\gamma\gamma}^{neq*} = \gamma_b \Pi_{\gamma\gamma}^{neq} = \gamma_b \sum_j n_j^{neq} c_{j\gamma} c_{j\gamma} = \sum_j (\gamma_b c_{j\gamma} c_{j\gamma}) n_j^{neq}$$

$$\gamma_b c_{j\gamma} c_{j\gamma} = \sum_i c_{i\gamma} c_{i\gamma} \Gamma_{ij}$$

$$e_{4i} := c_{i\gamma} c_{i\gamma}$$

$$e_{4j} \gamma_b = \sum_i e_{4i} \Gamma_{ij}$$

i. e.  $\vec{e}_4$  is left eigenvector, eigenvalue  $\gamma_b$

... and so on!  $\vec{e}_5, \dots, \vec{e}_9$ : five shear stresses, eigenvalue  $\gamma_s$  (same value for symmetry reasons)

$\vec{e}_{10}, \dots, \vec{e}_{18}$  9 “kinetic modes”, “ghost modes” (higher-order polynomials in the  $\vec{c}_i$ )

i. e. we do not know  $\Gamma$  directly, but its eigenvalues and eigenvectors!

generally (eigenvalues  $\gamma_i$ )

$$e_{kj}\gamma_k = \sum_i e_{ki}\Gamma_{ij}$$

$$|\gamma_i| \leq 1$$

for linear stability!

set

$$\begin{aligned}
 m_k &= \sum_j e_{kj} n_j \\
 m_k^{neq*} &= \sum_i e_{ki} n_i^{neq*} = \sum_i e_{ki} \sum_j \Gamma_{ij} n_j^{neq} \\
 &= \sum_j \left( \sum_i e_{ki} \Gamma_{ij} \right) n_j^{neq} = \sum_j e_{kj} \gamma_k n_j^{neq} = \gamma_k m_k^{neq}
 \end{aligned}$$

I. e. the relaxation process is simple in mode space!

- $\gamma_0 = \gamma_1 = \gamma_2 = \gamma_3 = 0$  (mass and momentum conservation)
- $\gamma_4 = \gamma_b$  (bulk stress)
- $\gamma_5 = \dots = \gamma_9 = \gamma_s$  (shear stress)
- $\gamma_{10} = \dots = \gamma_{18} = 0$  (simplest choice, not necessary)

scalar product:

$$\langle \vec{n}' | \vec{n} \rangle = \sum_i w_i n'_i n_i$$

**Claim:** It is possible to pick the eigenvectors in such a way that they satisfy

$$\langle \vec{e}_k | \vec{e}_l \rangle = \mathcal{N}_k \delta_{kl}$$

where the  $\mathcal{N}_k$  are just normalization constants.

**Proof:** Either you understand group theory pretty well, or you do an explicit Gram–Schmidt orthogonalization! Result is tabulated in the review!

$$\begin{aligned}
\delta_{kl} &= \frac{1}{\mathcal{N}_k} \sum_i w_i e_{ki} e_{li} \\
&= \sum_i \sqrt{\frac{w_i}{\mathcal{N}_k}} e_{ki} \sqrt{\frac{w_i}{\mathcal{N}_l}} e_{li} \\
\hat{e}_{ki} &:= \sqrt{\frac{w_i}{\mathcal{N}_k}} e_{ki} \\
\delta_{kl} &= \sum_i \hat{e}_{ki} \hat{e}_{li}
\end{aligned}$$

i. e.  $\hat{e}_{ki}$  is a standard orthogonal matrix with Euclidean scalar product!

$$\begin{aligned}
 m_k &= \sum_i e_{ki} n_i = \sum_i \sqrt{\frac{\mathcal{N}_k}{w_i}} \hat{e}_{ki} n_i \\
 \hat{m}_k &:= \frac{1}{\sqrt{\mathcal{N}_k}} m_k \\
 \hat{n}_i &:= \frac{1}{\sqrt{w_i}} n_i \\
 \hat{m}_k &= \sum_i \hat{e}_{ki} \hat{n}_i
 \end{aligned}$$

orthonormal transformation, trivial to invert!

$$\Pi_{\alpha\beta} = \bar{\Pi}_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta}\Pi_{\gamma\gamma}$$

$$\bar{\Pi}_{\alpha\beta}^{*neq} = \gamma_s \bar{\Pi}_{\alpha\beta}^{neq}$$

$$\bar{\Pi}_{\gamma\gamma}^{*neq} = \gamma_b \bar{\Pi}_{\gamma\gamma}^{neq}$$

$$\begin{aligned}\Pi_{\alpha\beta}^{*neq} - \Pi_{\alpha\beta}^{neq} &= \bar{\Pi}_{\alpha\beta}^{*neq} - \bar{\Pi}_{\alpha\beta}^{neq} + \frac{1}{3}\delta_{\alpha\beta}(\Pi_{\gamma\gamma}^{*neq} - \Pi_{\gamma\gamma}^{neq}) \\ &= (\gamma_s - 1)\bar{\Pi}_{\alpha\beta}^{neq} + \frac{1}{3}\delta_{\alpha\beta}(\gamma_b - 1)\Pi_{\gamma\gamma}^{neq}\end{aligned}$$

on the other hand, we had derived

$$\begin{aligned}\Pi_{\alpha\beta}^{*neq} - \Pi_{\alpha\beta}^{neq} &= h\rho c_s^2 (\partial_\alpha u_\beta + \partial_\beta u_\alpha) \\ &= h\rho c_s^2 \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ &\quad + \frac{2}{3} h\rho c_s^2 \delta_{\alpha\beta} \partial_\gamma u_\gamma\end{aligned}$$

comparison:

$$\begin{aligned}(\gamma_s - 1) \bar{\Pi}_{\alpha\beta}^{neq} &= h\rho c_s^2 \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ (\gamma_b - 1) \Pi_{\gamma\gamma}^{neq} &= 2h\rho c_s^2 \partial_\gamma u_\gamma\end{aligned}$$

or

$$\begin{aligned}\bar{\Pi}_{\alpha\beta}^{neq} &= \frac{h\rho c_s^2}{\gamma_s - 1} \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ \Pi_{\gamma\gamma}^{neq} &= \frac{2h\rho c_s^2}{\gamma_b - 1} \partial_\gamma u_\gamma\end{aligned}$$



Chapman–Enskog told us: Newtonian viscous stress is

$$-\sigma_{\alpha\beta} = \frac{1}{2} \left( \Pi_{\alpha\beta}^{neq*} + \Pi_{\alpha\beta}^{neq} \right)$$

hence

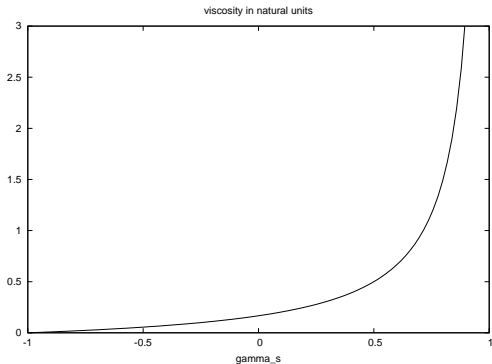
$$\begin{aligned} \frac{1}{2} \left( \bar{\Pi}_{\alpha\beta}^{neq*} + \bar{\Pi}_{\alpha\beta}^{neq} \right) &= \frac{1}{2} (\gamma_s + 1) \bar{\Pi}_{\alpha\beta}^{neq} \\ &= \frac{h\rho c_s^2}{2} \frac{\gamma_s + 1}{\gamma_s - 1} \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ &= -\eta \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \end{aligned}$$

and

$$\begin{aligned} \frac{1}{2} \frac{1}{3} \delta_{\alpha\beta} \left( \Pi_{\gamma\gamma}^{neq*} + \Pi_{\gamma\gamma}^{neq} \right) &= \frac{1}{2} \frac{1}{3} \delta_{\alpha\beta} (\gamma_b + 1) \Pi_{\gamma\gamma}^{neq} \\ &= \frac{h\rho c_s^2}{3} \frac{\gamma_b + 1}{\gamma_b - 1} \delta_{\alpha\beta} \partial_\gamma u_\gamma \\ &= -\zeta \delta_{\alpha\beta} \partial_\gamma u_\gamma \end{aligned}$$

read off viscosities:

$$\eta = \frac{h\rho c_s^2}{2} \frac{1 + \gamma_s}{1 - \gamma_s} \quad \zeta = \frac{h\rho c_s^2}{3} \frac{1 + \gamma_b}{1 - \gamma_b}$$



- $|\gamma_i| \leq 1 \Leftrightarrow$  positive viscosities!
- *any* viscosity values are accessible!